Directed Motion of Carbon Nanotube in Water Driven by Non-uniform Electric Field

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Summary Utilizing molecular dynamics simulations, we propose two designs to achieve the directed motions of the SWCNT in water environment by electric field with a linear gradient in the present study. The possible mechanism of the directed motion may be attributed to the non-uniform distribution of the interfacial hydrogen bonds along the SWCNT induced by the non-uniform electric field.

INTRODUCTION

Due to the quasi one-dimensional nature of the single-walled carbon nanotubes (SWCNTs), the SWCNTs are regarded as one of the promising and powerful tools for molecules transportation or mass delivery. The molecules or particles could be delivered either inside or outside the tube walls because of the tubular geometry of CNTs. In recent years, various driving force have been proposed to achieve the atomic scale mass transport along the SWCNT, such as the electromigration, pressure gradient and thermal gradient (thermophoresis).

Although the designs above-mentioned are fascinating and potentially applicable, seeking an alternative technique to fulfill the motion of CNT in aqueous environment gains increasing interests. Utilizing MD simulations, two kinds of assembly in aqueous environment for achieving the directed movements are proposed in the present study. The systems are consisted of two coaxial SWCNTs, i.e., a short SWCNT either outside (System 1, denoted by S1) or inside (System 2, denoted by S2) [Figure 1(a) and Figure 1(b)] a longer SWCNT. After the electric field with a linear gradient is applied, in S1 the outer short SWCNT moves moves to the area with lower field strength, while in S2 the inner capsule-like SWCNT travels in the opposite direction.

MODEL AND NUMERICAL METHOD

The sketches of the physical models considered in the present study are illustrated in Figure 1. For the S1, the inner one is 12.149 nm long with a chiral vector of (5,5) corresponding to a diameter of 0.678 nm, while the outer one is 1.858 nm long with a chiral vector of (10,10) corresponding to a diameter of 1.356 nm. The S2 consists of an outer 12.149 nm long (10,10) SWCNT and an inner capsule-like SWCNT modeled as an open short 1.858 nm long (5,5) SWCNT with caps on two ends. The two systems are placed in a cubic box with dimensions of $L_x = 6nm, L_y = 6nm$ and $L_z = 16nm$. The axes of the SWCNTs are along the Z-direction. Water molecules with the density 998 kg/m^3 are filled in the outer space of the SWCNTs. Then a non-uniform electric field with linear gradient is applied to the system. The direction of the electric field is along the X-direction and the strength is given by $E = E_z(z / L_z)$, where E_z is a constant controlling parameter with $0 \le E_z \le 4.8$ V/nm. The MD simulations are performed at a constant temperature 300K and pressure 1bar. All these parameters employed in the present study have been widely used in previous researches [1].

RESULTS AND DISCUSSION

Initially, the short SWCNTs are fixed by position restraint. Then both two systems are simulated for 1ns in the absence of electric field. Afterwards the position restraints of the short SWCNTs are removed, and the two systems are computed for an additional 5-8 ns with the linearly gradient electric field of E_Z = 0.8, 1.6, 3.2, 4.8 V/nm. During the simulations, the positions of the center of mass (COM) of the short SWCNTs are measured, which are shown in Figure 2(a) and 2(b). For the S1, the short (10,10) SWCNT moves to the area with lower field strength along the tube axis, and finally reaches the open end of the long (5,5) SWCNT. The short SWCNT can't escape from the long SWCNT because of the existence of the van der Waals potential energy barrier between the two SWCNTs. Because of the thermal motion induced by the interactions between short SWCNT and water molecules, apparent fluctuations can be found on the curves. For the S2, interestingly, the capsule-like (5,5) SWCNT moves to the area with higher field strength, along the direction opposite to the observation in the S1. When the capsule arrives at the open end of the long (10,10) SWCNT, it also keeps oscillating there and can't escape. As the capsule is confined in the interior of the long SWCNT, the thermal motion effects of the water molecules on it are very weak. Therefore the curve of the COM is much smoother than that in S1 and the motion is nearly steady in the sense of statistics.

It might be interesting to seek the physical mechanism behind these two types of nanomotors. In the present studies, the electric field applied is perpendicular to the nanotube axis and has a linear gradient. Previous studies have shown that

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the electric field along the nanotube axis has profound influence on water structures in the confinement. Luzar et al. [2-3] have reported that a freely rotating nanoparticle in water in the presence of electric field could be aligned through water mediation. The major contributions to the torque come from two effects which are the preference of water to maximize its hydrogen bonds and the tendency of water to polarize parallel to the interface. Herein, the similar effects may be employed for our nanomotors. The average number of hydrogen bonds per water molecule $<n_{HB}>$ in the vicinity of the SWCNT walls is presented in Figure 3 as a function of the strength of the electric field. It is interesting to find that, as the field strength increasing, more hydrogen bonds are formed outside the (5,5) SWCNT, which is shown in Figure 3(a). That is to say, in the S1, along the axis direction of (5,5) long SWCNT, more hydrogen bonds should be formed in the interface with higher field strength in the absence of the short SWCNT. When the short (10,10) SWCNT is placed at the location with higher field strength, the equilibrium state of the hydrogen bonds at the interface will be destroyed. Therefore, the short (10,10) SWCNT has to move to the area with less interface hydrogen bonds, trying to maximize the average hydrogen bonds. The similar tendency is also observed in the S2. In Figure 3(b), for (10,10) SWCNT, the $<n_{HB}>$ inside these SWCNTs decreases as the field strength increases. As we have known, the capsule-like capped (5,5) SWCNT moves to the area with higher field strength, which leads to the formation of more hydrogen bonds inside the long (10,10) SWCNT. To confirm these results, the systems consisting of (6,6) and (8,8) SWCNTs are also simulated and same conclusions are drawn in the present study.

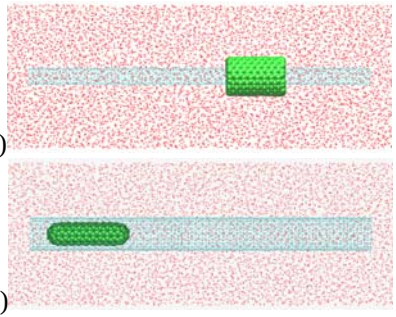
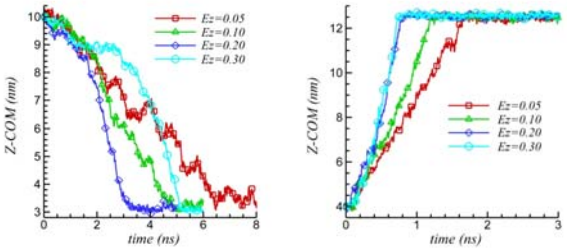
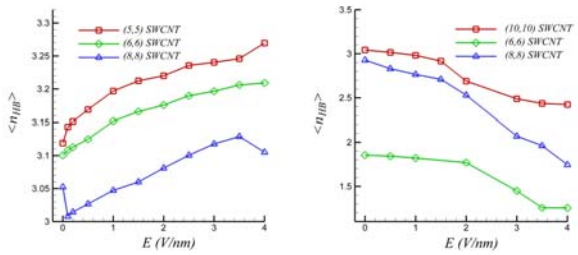


Figure 1. The sketches of physical models of (a) S1 and (b) S2.



(a) (b)

Figure 2. The COM of the short SWCNTs of (a) S1 and (b) S2 with E_z= 0.05, 0.10, 0.20 and 0.30 V/nm.



(a) (b)

Figure 3. The variation of the average number of hydrogen bonds per water molecule $<n_{HB}>$ in vicinity of the interface of with the diameter of long SWCNT. (a) S1 for (5,5), (6,6) and (8,8) SWCNTs, (b) S2 for (6,6), (8,8) and (10,10) SWCNTs.

CONCLUSIONS

The molecular dynamics simulations are performed to demonstrate that in aqueous environment, a short (10,10) SWCNT outside a long (5,5) SWCNT or a capsule-like (5,5) SWCNT inside a long (10,10) SWCNT is capable of moving along the nanotube axis unidirectionally under the electric field with linear gradient. Results show that the short (10,10) SWCNT moves to the area with lower field strength while the capsule moves to the area with higher field strength. The preference of water to maximize its hydrogen bonds and the tendency of water to polarize parallel to the interface in the presence of electric field may be the major contribution to the driving force. We find that the hydrogen bonds outside the SWCNT increase as the field strength increasing whereas the tendency is opposite inside the SWCNT.

References

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